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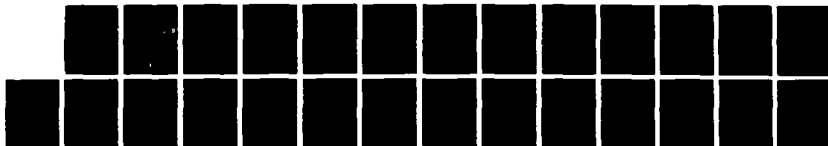
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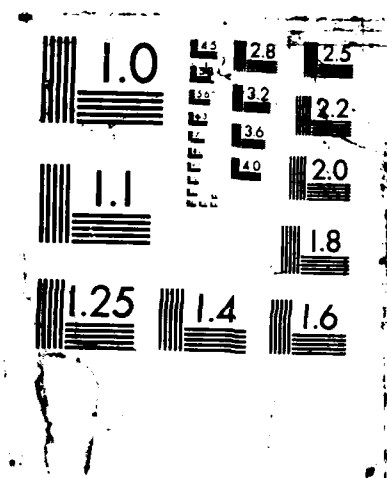
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by

Mark Knowles and David Siegmund  
Alza Corporation and Stanford University

TECHNICAL REPORT NO. 6  
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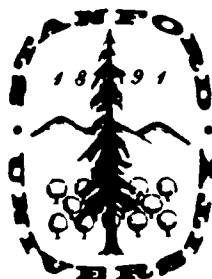
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DEPARTMENT OF STATISTICS  
STANFORD UNIVERSITY  
STANFORD, CALIFORNIA

# On Hotelling's Approach to Testing for a Nonlinear Parameter in Regression

by

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## Abstract.

The method suggested by Hotelling (1939) to test for a nonlinear parameter in a regression model is reviewed. Using the method of Weyl (1939), we derive a simple expression for the volume of a tube about a two dimensional manifold with boundary embedded in the unit sphere in  $\mathbb{R}^n$ . Applications to testing for a single harmonic of undetermined frequency and phase and to testing for a change-point in linear regression are discussed.

Key words: Tube volume, nonlinear regression, differential geometry.

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## 1. Introduction.

Hotelling (1939) and Weyl (1939) initiated a profound line of geometric research (e.g. Griffiths, 1978, Langevin and Shifrin, 1982, Gray, 1982), motivated by the following statistical question. Suppose  $y_i = \beta f_i(\theta) + \varepsilon_i$  ( $i = 1, 2, \dots, n$ ), where the  $f_i$  are known functions depending on an unknown, perhaps multidimensional parameter  $\theta$ , and the  $\varepsilon_i$  are independent  $N(0, \sigma^2)$  errors. What is the significance level of the likelihood ratio test of  $H_0 : \beta = 0$ ? (One can also consider the more general model  $y_i = \langle \alpha, x_i \rangle + \beta f_i(\theta) + \varepsilon_i$ , where  $\alpha$  is a  $p$ -dimensional parameter and the  $x_i$  are known  $p$ -dimensional vectors, as we show in Section 4.)

One of Hotelling's principal motivating examples is  $f_i(\theta) = \cos(\mu t_i + \omega)$ , where the  $t_i$  are known constants and  $\theta = (\mu, \omega)$ . Another example is the broken line regression  $f_i(\theta) = (t_i - \theta)^+$ . Davies (1987) gives an interesting discussion of each of these problems from a different viewpoint.

It is easy to see that the likelihood ratio statistic for testing  $H_0 : \beta = 0$  is equivalent to

$$\max_{\theta} \left\{ [\Sigma f_i(\theta) y_i]^2 / [\Sigma f_i^2(\theta) \Sigma y_i^2] \right\}.$$

Setting  $f(\theta) = (f_1(\theta), \dots, f_n(\theta))$  and  $y = (y_1, \dots, y_n)$ , we can write this statistic in the form

$$\max_{\theta} \left\{ \langle f(\theta), y \rangle^2 / [\|f(\theta)\|^2 \|y\|^2] \right\}.$$

In terms of the unit vectors  $\gamma(\theta) = f(\theta)/\|f(\theta)\|$  and  $U = y/\|y\|$ , the rejection region is of the form

$$\max_{\theta} \langle \gamma(\theta), U \rangle^2 \geq w^2.$$

The rejection region can be described geometrically as the union of two tubes in the unit sphere  $S^{n-1}$ , one about  $\gamma(\theta)$  and one about  $-\gamma(\theta)$ , of geodesic radius  $\cos^{-1}(w)$ . Here the tube about  $\gamma(\theta)$  of geodesic radius  $\varphi$  is the set of all  $u \in S^{n-1}$  within geodesic distance  $\varphi$  of the manifold  $\gamma(\theta)$  as  $\theta$  ranges over some parameter space. Under  $H_0$   $U$  is distributed uniformly on  $S^{n-1}$  and hence the significance level of the likelihood ratio test is the normalized surface area on  $S^{n-1}$  of the union of the two tubes.

The purpose of this paper is to review the Hotelling-Weyl approach and explore its statistical implications by a detailed discussion of the two concrete examples mentioned above. Additional applications are described by Naiman (1986a,b), Knowles (1986), and Johansen and Johnstone (1988).

The theoretical basis for our discussion of the broken line regression, which involves a one dimensional parameter  $\theta$ , is given by Naiman (1986) and Johnstone and Siegmund (1987). The

theoretical situation for multidimensional  $\theta$  is less satisfactory. Since Weyl's theorem concerns manifolds without boundary whereas many statistical problems and Hotelling's example in particular involve manifolds with boundary, we begin by giving a version of Weyl's theorem for two dimensional manifolds (surfaces) with boundary embedded in  $S^{n-1}$ . The two dimensional case is especially interesting because a term which would be onerous to evaluate numerically can be combined with other terms and evaluated analytically by an application of the Gauss-Bonnet Theorem. Naiman (1987) discusses a special class of  $d$ -dimensional manifolds with boundary, but even in the case  $d = 2$  his result is somewhat differently formulated.

Our numerical studies have two purposes. (i) Since the Hotelling-Weyl theory is exact only for tubes of small radii, i.e. for small significance levels, we indicate through these concrete examples the accuracy provided by the theoretical results at conventional significance levels. (ii) Since the theoretical results contain coefficients depending on the sample size and dimension of the parameter space, which can be difficult to compute, we investigate numerically the effect of approximating or neglecting some of these coefficients.

The paper is organized as follows. Section 2 contains our version of Weyl's theorem for surfaces with boundary. Once the theorem is formulated the proof is not difficult for the careful reader of Weyl's paper. Nevertheless, we give the argument in some detail because the restriction to surfaces makes possible a completely elementary (in the sense of differential geometry) exposition, which we hope will make the subject more widely known by statisticians. Section 3 specializes our general theorem to the problem of testing for a periodic term and compares some numerical results with the outcomes of a simulation experiment. Section 4 discusses the problem of testing for a break in a regression line. For the most part Sections 3 and 4 can be read independently of Section 2. In Section 5 we try to draw some qualitative conclusions and discuss possible extensions of our results.

## 2. The Volume of Tubes about Surfaces with Boundary.

Suitable references for the following developments are Millman and Parker (1977) and Do Carmo (1976). The former is notationally consistent with Weyl (1939) and with modern usage, and consequently that notation is used here. The latter gives a more thorough and often more adequate treatment of the concepts needed below.

As in Hotelling (1939) and Weyl (1939) we consider first the technically simpler case of surfaces  $M$  in  $\mathbb{R}^n$  and then indicate the modifications required for surfaces in the unit sphere  $S^{n-1} \subset \mathbb{R}^n$ .

We assume that a regular, oriented surface  $M \subset \mathbb{R}^n$  is given locally by a  $C^3$  function

$x = x(u^1, u^2)$  defined on an open set in  $\mathbb{R}^2$ . Assume also that the boundary of  $M$ , say  $\partial M$ , is given by a piecewise regular, positively oriented curve  $\gamma$ , parameterized by arc length. (The reader who wishes to avoid the technical concept of orientation may consider the special case in which  $M$  is given globally by  $x(u^1, u^2)$ .)

The tube about  $M$  of radius  $a$  is the set of all points whose minimum distance to  $M$  is less than  $a$ . We say that overlap occurs at a point  $y$  in the tube if there exists more than one point in the manifold which is closest to  $y$ .

Let  $|M|$  and  $|\partial M|$  denote the surface area of  $M$  and length of  $\partial M$  respectively. Let  $\Omega_n$  denote the volume of the unit ball in  $\mathbb{R}^n$  and  $\omega_n$  the volume (surface area) of the unit sphere  $S^n \subset \mathbb{R}^{n+1}$  ( $\Omega_n = \pi^{n/2}/\Gamma(n/2 + 1)$ ,  $\omega_{n-1} = 2\pi^{n/2}/\Gamma(n/2)$ ; our  $\omega_{n-1}$  is Weyl's  $\omega_n$ ).

**Theorem 1.** Assume that the exterior angles at the vertices (if any) of  $\partial M$  are positive in the sense that the tangent to  $\gamma$  rotates through a positive angle at each vertex. For all  $a$  sufficiently small that no overlap occurs in the tube of radius  $a$  about  $M$ , the volume  $V(a)$  of the tube is given by

$$V(a) = |M|\Omega_{n-2}a^{n-2} + 2^{-1}|\partial M|\Omega_{n-1}a^{n-1} + 2\pi\chi(M)\Omega_{n-2}a^n/n, \quad (1)$$

where  $\chi(M)$  is the Euler-Poincaré characteristic of  $M$ .

**Remarks.** (i) the factor  $2\pi\chi(M)$  in (1) arises indirectly as

$$\int_M K dA + \int_{\partial M} k_g ds + \sum \theta_i, \quad (2)$$

where  $K$  is the Gaussian curvature and  $dA$  the element of surface area of  $M$ ,  $k_g$  is the geodesic curvature and  $ds$  the element of arc length of  $\partial M$ , and the  $\theta_i$  are the angles of rotation of the tangent to  $\gamma(s)$  at the vertices of  $\partial M$ . That (2) equals  $2\pi\chi(M)$  is the Gauss-Bonnet Theorem (Do Carmo, 1976, p. 274). Since numerical evaluation of the individual terms in (2) would be onerous whereas  $\chi(M)$  is easily determined and in statistical problems is often zero or one, this simplification of (2) is quite fortunate. That the various ingredients of (2) are involved in  $V(a)$  is not surprising. That they all have the same coefficient and hence can be combined appears in our proof as an accident of calculation for which we do not have a satisfactory geometric explanation.

(ii) The condition that no overlap occurs is both a local and a global condition. The tube overlaps itself locally whenever one of the Jacobian matrices appearing in the following argument



has a vanishing determinant. In that case the curvature of the surface is so great that the mapping which parameterizes points in the tube is not locally one-to-one. The occurrence of global overlap is not so easily characterized. If no local overlap occurs, the right hand side of (1) is an upper bound for the left hand side. Johansen and Johnstone (1988) give an algorithm to determine the smallest radius at which overlap occurs in a tube about a curve.

(iii) If some of the exterior angles at vertices of  $\partial M$  are negative and no self overlap occurs except the local self overlap at those vertices,  $V(a)$  is  $\leq$  the right hand side of (1).

**Proof.** We give the proof for  $n = 4$ , which simplifies the necessary computations and except for one technical identity given at the end of the proof has all the ingredients of the general case. The method involves evaluation of the differential of volume at a point  $y$  in the tube, say  $dV(y)$ , followed by integration over the tube. We consider separately the case of points  $y$  which are nearest an interior point of  $M$  and points nearest to a boundary point. Initially we follow Weyl closely.

For points  $y$  nearest to an interior point  $x = x(u^1, u^2)$  we have  $y = x + \xi_1 n(1) + \xi_2 n(2)$ , where  $n(1)$  and  $n(2)$  are mutually orthogonal unit normals to the tangent space to  $M$  at  $x(u^1, u^2)$ . Then  $y = y(u^1, u^2, \xi_1, \xi_2)$  and

$$dV(y) = \|y_1, y_2, y_3, y_4\| du^1 du^2 d\xi_1 d\xi_2, \quad (3)$$

where  $y_i$  denotes the partial derivative of  $y$  with respect to the  $i^{\text{th}}$  argument, and the double bars denote the absolute value of the determinant of the Jacobian matrix of the enclosed (column) vectors. We have

$$\begin{aligned} y_i &= x_i + \xi_1 n_i(1) + \xi_2 n_i(2) \quad (i = 1, 2), \\ y_3 &= n(1), y_4 = n(2), \end{aligned} \quad (4)$$

where  $x_i = \partial x / \partial u^i$  and  $n_i(\nu) = \partial n(\nu) / \partial u^i$ . We can express  $n_i(\nu)$  as a linear combination of  $x_1, x_2, n(1)$ , and  $n(2)$  by (Weingarten equations)

$$n_i(\nu) = -\sum_j L_i^j(\nu) x_j + \dots, \quad (5)$$

where  $-L_i^j(\nu)$  is for our purposes defined to be the coefficient of  $x_j$  in the indicated expansion, and  $+\dots$  indicates components orthogonal to the tangent space spanned by  $x_1$  and  $x_2$ . Hence writing

$$L(\nu) = \begin{pmatrix} L_1^1(\nu) & L_1^2(\nu) \\ L_2^1(\nu) & L_2^2(\nu) \end{pmatrix},$$

we have in matrix form by (4) and (5)

$$(y_1, y_2) = (x_1, x_2)(I - \xi_1 L(1) - \xi_2 L(2)) + \dots,$$

so (3) becomes

$$\begin{aligned} dV(y) &= \|(x_1, x_2)(I - \xi_1 L(1) - \xi_2 L(2)), n(1), n(2)\| du^1 du^2 d\xi_1 d\xi_2 \\ &= \|x_1, x_2, n(1), n(2)\| \|I - \xi_1 L(1) - \xi_2 L(2)\| du^1 du^2 d\xi_1 d\xi_2. \end{aligned} \quad (6)$$

From the determinantal identity

$$|v_1, \dots, v_k|^2 = |\langle v_i, v_j \rangle|,$$

we see that the first factor on the right hand side of (6) equals  $g^{1/2}$ , where  $(g_{ij}) = (\langle x_i, x_j \rangle)$  is the matrix of the first fundamental form of  $M$  and  $g = |g_{ij}|$ . Since  $dA = g^{1/2} du^1 du^2$  is the element of surface area on  $M$ , we see from (6) that the volume associated with points  $y$  closest to interior points of  $M$  is

$$V_1(a) = \int_M \iint_{\xi_1^2 + \xi_2^2 \leq a^2} |I - \xi_1 L(1) - \xi_2 L(2)| d\xi_1 d\xi_2 dA. \quad (7)$$

Expansion of the determinant in (7) yields

$$\begin{aligned} &1 - \xi_1 \text{tr } L(1) - \xi_2 \text{tr } L(2) + \xi_1^2 |L(1)| + \xi_2^2 |L(2)| \\ &+ \xi_1 \xi_2 \{L_1^1(1) L_2^2(2) + L_1^1(2) L_2^2(1) - 2L_2^1(1) L_1^1(2)\}, \end{aligned}$$

so

$$\begin{aligned} V_1(a) &= \int_M \int_{\xi_1^2 + \xi_2^2 \leq a^2} (1 + \xi_1^2 |L(1)| + \xi_2^2 |L(2)|) d\xi_1 d\xi_2 dA \\ &= \pi a^2 |M| + \int_M (|L(1)| + |L(2)|) \int_{\xi_1^2 + \xi_2^2 \leq a^2} \xi_1^2 d\xi_1 d\xi_2 dA \\ &= \pi a^2 |M| + 4^{-1} \pi a^4 \int_M (|L(1)| + |L(2)|) dA. \end{aligned}$$

To identify  $|L(1)| + |L(2)|$  as the Gaussian curvature  $K$ , we put  $x_{ij} = \partial x / \partial u^i \partial u^j$  and in the customary way (e.g. Do Carmo, 1976, p. 232) define Christoffel symbols  $\Gamma_{ij}^k$  and coefficients  $L_{ij}(\nu)$  by

$$x_{ij} = \sum_k \Gamma_{ij}^k x_k + \sum_\nu L_{ij}(\nu) n(\nu).$$

Since  $\langle x_i, n(\nu) \rangle = 0$ ,  $L_{ij}(\nu) = \langle x_{ij}, n(\nu) \rangle = -\langle x_i, n_j(\nu) \rangle$ , and hence by (5)  $L_{ij}(\nu) = \sum_k g_{ik} L_j^k(\nu)$ . One can now proceed line by line as in standard proofs of Gauss's *Theorema Egregium* (e.g. Do Carmo, 1976, pp. 233-34; Millman and Parker, 1977, pp. 142-43) to show that the intrinsic evaluation of  $K$  in terms of the Christoffel symbols and their partial derivatives

equals  $|L(1)| + |L(2)|$ . Hence

$$V_1(a) = \pi a^2 |M| + 4^{-1} \pi a^4 \int_M K dA. \quad (8)$$

Now assume that the closest point in  $M \cup \partial M$  to  $y$  is a point  $\gamma(s) \in \partial M$  where  $\dot{\gamma}(s) = d\gamma/ds$  exists. Then

$$y = \gamma + \eta n(0) + \xi_1 n(1) + \xi_2 n(2), \quad (9)$$

where  $n(0)$  is a unit vector in the tangent plane of  $M$ , but orthogonal to  $\dot{\gamma}$  and as before  $n(1)$  and  $n(2)$  are orthogonal to the tangent plane. We choose  $n(0)$  to point towards the interior of the manifold (rotated by  $+\pi/2$  from  $\dot{\gamma}$ ), so the geodesic curvature  $k_g = k_g(s) = \langle \ddot{\gamma}, n(0) \rangle$ , and  $\eta \in (-a, 0]$ .

The volume element is

$$dV(y) = \|y_1, y_2, y_3, y_4\| ds d\eta d\xi_1 d\xi_2,$$

where as before  $y_i$  is the partial derivative of  $y = y(s, \eta, \xi_1, \xi_2)$  with respect to the  $i^{\text{th}}$  argument. Putting  $\dot{q} = dq/ds$ , we have the Frenet-Serret equations (cf. Do Carmo, 1976, p. 261)

$$\begin{aligned} \ddot{\gamma} &= k_g n(0) + k_1 n(1) + k_2 n(2) \\ \dot{n}(0) &= -k_g \dot{\gamma} + \tau_1 n(1) + \tau_2 n(2) \\ \dot{n}(1) &= -k_1 \dot{\gamma} - \tau_1 n(0) + \tau_3 n(2) \\ \dot{n}(2) &= -k_2 \dot{\gamma} - \tau_2 n(0) - \tau_3 n(1), \end{aligned}$$

where except for  $k_g$  the values of the coefficients ultimately will not concern us. Hence by (9)

$$\begin{aligned} dV &= \|\dot{\gamma} + \eta \dot{n}(0) + \xi_1 \dot{n}(1) + \xi_2 \dot{n}(2), n(0), n(1), n(2)\| ds d\eta d\xi_1 d\xi_2 \\ &= \|\dot{\gamma}(1 - \eta k_g - \xi_1 k_1 - \xi_2 k_2), n(0), n(1), n(2)\| ds d\eta d\xi_1 d\xi_2. \end{aligned}$$

The volume associated with these points  $y$  is

$$\begin{aligned} V_2(a) &= \int_{\partial M} \iiint_{\substack{\eta \leq 0 \\ \eta^2 + \xi_1^2 + \xi_2^2 \leq a^2}} (1 - \eta k_g - k_1 \xi_1 - k_2 \xi_2) d\xi_1 d\xi_2 d\eta ds \\ &= \int_{\partial M} \int_{-a}^0 \pi(a^2 - \eta^2)(1 - k_g \eta) d\eta ds \\ &= 2\pi |\partial M| a^3/3 + 4^{-1} \pi a^4 \int_{\partial M} k_g ds. \end{aligned} \quad (10)$$

The contribution to  $V(a)$  from points in the tube which are closest to vertices of  $\partial M$  is clearly

$$V_3(a) = \Omega_4 a^4 \Sigma \theta_i / 2\pi = 4^{-1} \pi a^4 \Sigma \theta_i, \quad (11)$$

where the  $\theta$ 's are the angles of rotation of the tangent to  $\gamma$  at the vertices.

Addition of (8), (10), and (11) and an appeal to the Gauss-Bonnet Theorem as indicated in Remark (i) following the statement of the theorem complete the proof in the special case  $n = 4$ .

The proof for general  $n$  is essentially the same. The coefficients of  $\int_M K dA$ ,  $\int_{\partial M} k_g ds$ , and  $\Sigma \theta_i$  are respectively

$$a^n \int \dots \int_{\xi_1^2 + \dots + \xi_{n-2}^2 \leq 1} \xi_1^2 d\xi_1, \dots, d\xi_{n-2}, -a^n \int \dots \int_{\substack{\eta \leq 0 \\ \eta^2 + \xi_1^2 + \dots + \xi_{n-2}^2 \leq 1}} \eta d\eta d\xi_1 \dots d\xi_{n-2},$$

and  $(2\pi)^{-1} a^n \Omega_n$ , which some calculus shows are all equal to  $n^{-1} a^n \Omega_{n-2}$ . ■

To prepare for the spherical case suppose  $y = y(u^1, \dots, u^{n-1})$  is a coordinate patch of a hypersurface in  $\mathbb{R}^n$ . Let  $\rho = \langle y, y \rangle$  and  $z = y/\rho \in S^{n-1}$ . Assume  $z$  is one-to-one.

**Lemma 1** (Weyl): The volume element at  $z \in S^{n-1}$  is given by

$$dV(z) = \|y, y_1, \dots, y_{n-1}\| du^1 \dots du^{n-1} / \rho^n,$$

where  $y_i = \partial y / \partial u^i$ .

**Proof.** Since  $z$  is the unit normal to the hypersurface  $z(u^1, \dots, u^{n-1})$ ,

$$dV(z) = \|z, z_1, \dots, z_{n-1}\| du^1 \dots du^{n-1},$$

where  $z_i = \partial z / \partial u^i$ . Since

$$z_i = \rho^{-1} y_i + y \partial \rho^{-1} / \partial u^i,$$

by collinearity we have  $|z, z_1, \dots, z_{n-1}| = |y, y_1, \dots, y_{n-1}| / \rho^n$ . ■

Now suppose  $M \subset S^{n-1}$ , the unit sphere in  $\mathbb{R}^n$ . The tube about  $M$  of geodesic radius  $\varphi$  is defined as the set of all  $z \in S^{n-1}$  such that  $\langle z, x \rangle > \cos \varphi$  for some  $x \in M$ .

**Theorem 2.** Assume that  $M \subset S^{n-1}$  and the exterior angles at the vertices of  $\partial M$  are positive. For all  $\varphi$  sufficiently small that no overlap occurs in  $S^{n-1}$  in the tube of geodesic radius  $\varphi$  about  $M$ , the volume  $V(\varphi)$  of the tube is given by

$$V(\varphi) = (n-3)^{-1} \omega_{n-4} [|M| \cos \varphi (\sin \varphi)^{n-3} + 2\pi \chi(M) \int_0^\varphi (\sin \omega)^{n-2} d\omega] + [2(n-2)]^{-1} \omega_{n-3} |\partial M| (\sin \varphi)^{n-2},$$

where  $\chi(M)$  is the Euler-Poincaré characteristic of  $M$ .

**Proof.** Suppose  $z$  is a point in the tube closest to an interior point  $x$  of  $M$ . Put  $k = n - 3$  and

$$y = y(u^1, u^2, \xi_1, \dots, \xi_k) = x + \xi_1 n(1) + \dots + \xi_k n(k), \quad (13)$$

where  $x = x(u^1, u^2) \in M$  and the  $n(\nu) \in S^{n-1}$  are mutually orthogonal unit normals to the tangent space of  $M$  at  $x(u^1, u^2)$ . Then we have the representation

$$z = y / (1 + \xi_1^2 + \dots + \xi_k^2)^{1/2},$$

where

$$\xi_1^2 + \dots + \xi_k^2 \leq \tan^2 \varphi.$$

By Lemma 1 and (13)

$$dV(z) = \|y, y_1, y_2, n(1), \dots, n(k)\| \frac{du^1 du^2 d\xi_1 \dots d\xi_k}{(1 + \xi_1^2 + \dots + \xi_k^2)^{n/2}}.$$

The proof of Theorem 1 together with some calculation shows that the contribution to the volume of the tube from these points is

$$\begin{aligned} V_1(\varphi) &= \int_M \int_{\sum_1^k \xi_i^2 \leq \tan^2 \varphi} (1 + \xi_1^2 \sum_1^k |L(\nu)|) \frac{d\xi_1 \dots d\xi_k}{(1 + \xi_1^2 + \dots + \xi_k^2)^{n/2}} dA \\ &= \omega_{n-4} [|M| \int_0^\varphi \cos^2 \omega (\sin \omega)^{n-4} d\omega \\ &\quad + (n-3)^{-1} \int_M (K-1) dA \int_0^\varphi (\sin \omega)^{n-2} d\omega] \\ &= (n-3)^{-1} \omega_{n-4} [|M| \cos \varphi (\sin \varphi)^{n-3} + \int_M K dA \int_0^\varphi (\sin \omega)^{n-2} d\omega]. \end{aligned} \quad (14)$$

The reason for the appearance of  $K-1$  in an intermediate equality of (14) is that (13) involves  $k = n - 3$  of the  $n - 2$  normals (in  $\mathbb{R}^n$ ) to the tangent space of  $M$ . The last normal is  $z$ , the normal to  $S^{n-1}$  itself. Its contribution to the (intrinsic) Gaussian curvature of  $M$  equals the Gaussian curvature of  $S^{n-1}$ , which is one. Hence from the  $n - 3$  normals represented in (13) we obtain  $K - 1$ .

For points  $z$  closest to a point of  $\partial M$  where  $\dot{\gamma}(s)$  exists, we have

$$y = \gamma + \eta n(0) + \xi_1 n(1) + \dots + \xi_k n(k), \quad z = y / (1 + \eta^2 + \xi_1^2 + \dots + \xi_k^2)^{1/2},$$

where  $n(0)$  is orthogonal to  $\dot{\gamma}$  but in the tangent space of  $M$  (pointing into  $M$ ), and  $n(1), \dots,$

$\eta(k)$  are as before. Also  $\eta \leq 0$  and  $\eta^2 + \xi_1^2 + \dots + \xi_k^2 \leq \tan^2 \varphi$ . By Lemma 1

$$\begin{aligned} dV(z) &= \|y, y_1, \dots, y_{n-1}\| \frac{ds d\eta d\xi_1 \dots d\xi_k}{(1 + \eta^2 + \xi_1^2 + \dots + \xi_k^2)^{n/2}} \\ &= \|\gamma, \dot{\gamma} + \eta \dot{n}(0) + \sum \xi_i \dot{n}(i), n(0), n(1), \dots, n(k)\| \frac{ds d\eta d\xi_1 \dots d\xi_k}{(1 + \eta^2 + \xi_1^2 + \dots + \xi_k^2)^{n/2}}. \end{aligned}$$

Using the Frenet-Serret equations as in the proof of Theorem 1, we obtain

$$dV(z) = (1 - k_g \eta - \sum_{i=1}^k c_i \xi_i) \frac{ds d\eta d\xi_1 \dots d\xi_k}{(1 + \eta^2 + \xi_1^2 + \dots + \xi_k^2)^{n/2}},$$

where  $k_g = \langle \ddot{\gamma}, n(0) \rangle = -\langle \dot{\gamma}, \dot{n}(0) \rangle$  is the geodesic curvature of  $\gamma$ , and the exact values of the coefficients  $c_i$  need not concern us. Hence the contribution to the volume of the tube arising from these points is

$$\begin{aligned} V_2(\varphi) &= \int_{\partial M} \int_{\substack{\eta \leq 0 \\ \eta^2 + \xi_1^2 + \dots + \xi_k^2 \leq \tan^2 \varphi}} (1 - k_g \eta) \frac{d\eta d\xi_1 \dots d\xi_k ds}{(1 + \eta^2 + \xi_1^2 + \dots + \xi_k^2)^{n/2}} \\ &= [2(n-2)]^{-1} \omega_{n-3} |\partial M| (\sin \varphi)^{n-2} + (n-3)^{-1} \omega_{n-4} \int_{\partial M} k_g ds \int_0^\varphi (\sin \omega)^{n-2} d\omega. \end{aligned} \quad (15)$$

Finally, the contribution arising from points nearest to a vertex of  $\partial M$  is

$$V_3(\varphi) = (n-3)^{-1} \omega_{n-4} (\sum \theta_i) \int_0^\varphi (\sin \omega)^{n-2} d\omega. \quad (16)$$

Addition of (14), (15), and (16) and an appeal to the Gauss-Bonnet Theorem as in Remark (i) following the statement of Theorem 1 complete the proof. ■

**Corollary 1.** Under the conditions of Theorem 2, if  $U$  is uniformly distributed on  $S^{n-1}$ ,

$$\begin{aligned} P\left\{ \sup_{u^1, u^2} \langle x(u^1, u^2), U \rangle > w \right\} &= \frac{2^{-1} \Gamma(n/2) |M| w (1 - w^2)^{\frac{n-3}{2}}}{\pi^{3/2} \Gamma[(n-1)/2]} \\ &\quad + (4\pi)^{-1} |\partial M| (1 - w^2)^{(n-2)/2} + \frac{\Gamma(n/2) \lambda(M)}{\pi^{1/2} \Gamma[(n-1)/2]} \int_w^1 (1 - x^2)^{(n-3)/2} dx. \end{aligned}$$

**Proof.** The corollary follows from the fact that the indicated probability is the normalized volume of the tube of geodesic radius  $\varphi = \cos^{-1} w$ , i.e.

$$V(\cos^{-1} w) / \omega_{n-1}.$$

### 3. Testing for an Harmonic.

Assume  $y_i = \beta \cos(\mu t_i + \omega) + \varepsilon_i$  ( $i = 1, 2, \dots, n$ ), where the  $t_i$  are known constants and the  $\varepsilon_i$  are independent  $N(0, \sigma^2)$ . The parameters  $\beta, \mu, \omega$ , and  $\sigma^2$  are all unknown, and we wish to test  $H_0 : \beta = 0$  against  $H_1 : \beta \neq 0$ . It is convenient to write

$$\beta \cos(\mu t_i + \omega) = \beta_1 \cos(\mu t_i) + \beta_2 \sin(\mu t_i),$$

where  $\beta_1 = \beta \cos \omega, \beta_2 = -\beta \sin \omega$ , and consider the equivalent problem of testing  $H_0 : \beta_1 = \beta_2 = 0$ . A calculation shows that the likelihood ratio test has a rejection region of the form

$$\sup_{\mu_1 < \mu < \mu_2} [\langle \gamma^1(\mu), U \rangle^2 + \langle \gamma^2(\mu), U \rangle^2]^{1/2} > w, \quad (17)$$

where  $\gamma^i(\mu) \in S^{n-1}, \langle \gamma^1(\mu), \gamma^2(\mu) \rangle = 0$  for all  $\mu$ , and  $U = y/\|y\|$  is uniformly distributed on  $S^{n-1}$  if  $H_0$  is true. In the special case that the  $t_i$  are equally spaced, the natural range of  $\mu$  is  $(0, \pi)$ .

Johnstone and Siegmund (1987) exploit the one dimensional structure of (17) and obtain by a non-geometric argument an upper bound for the significance level of the likelihood ratio test. We shall show as an application of Corollary 1 that their inequality is an equality when the significance level is sufficiently small. We also show by a Monte Carlo experiment that when the  $t_i$  are equally spaced these analytic results provide very good approximations for the true significance level over a broad range of values.

Note that

$$\begin{aligned} [\langle \gamma^1(\mu), U \rangle^2 + \langle \gamma^2(\mu), U \rangle^2]^{1/2} &= \sup_{0 \leq \omega < 2\pi} [\langle \gamma^1, U \rangle \cos \omega + \langle \gamma^2, U \rangle \sin \omega] \\ &= \sup_{0 \leq \omega < 2\pi} [\langle \gamma^1 \cos \omega + \gamma^2 \sin \omega, U \rangle]. \end{aligned}$$

Hence, if we put  $x(\mu, \omega) = \gamma^1(\mu) \cos \omega + \gamma^2(\mu) \sin \omega$ , Corollary 1 gives us the probability of (17) in terms of

$$\begin{aligned} |M| &= \int_0^{2\pi} \int_{\mu_1}^{\mu_2} \left[ \left\| \frac{\partial x}{\partial \mu} \right\|^2 \left\| \frac{\partial x}{\partial \omega} \right\|^2 - \left\langle \frac{\partial x}{\partial \mu}, \frac{\partial x}{\partial \omega} \right\rangle^2 \right]^{1/2} d\mu d\omega, \\ |\partial M| &= \int_0^{2\pi} \left\| \frac{\partial x(\mu_1, \omega)}{\partial \omega} \right\| d\omega + \int_0^{2\pi} \left\| \frac{\partial x(\mu_2, \omega)}{\partial \omega} \right\| d\omega, \end{aligned}$$

and  $\chi(M)$ .

Since  $\|\partial x / \partial \omega\| \equiv 1$  for all  $\mu$ ,  $|\partial M| = 4\pi$ . It is easy to see that  $\chi(M) = 0$ . For example, one can cut the surface along  $\omega = 0$  to obtain a new surface which clearly has Euler-Poincaré

characteristic equal to one and a connected boundary with four  $90^\circ$  exterior angles. Comparison of the Gauss-Bonnet Theorem applied to the cut and uncut surfaces shows that  $\chi(M) = 0$ .

To obtain an expression for  $|M|$ , observe that  $x_\omega = \partial x / \partial \omega = -\gamma^1 \sin \omega + \gamma^2 \cos \omega$  and  $x_\mu = \partial x / \partial \mu = \dot{\gamma}^1 \cos \omega + \dot{\gamma}^2 \sin \omega$ , so  $\|x_\omega\| \equiv 1$  and  $\|x_\mu\| = \|\dot{\gamma}^1 \cos \omega + \dot{\gamma}^2 \sin \omega\|$ . Since  $\langle \gamma^1, \gamma^2 \rangle = 0$ ,  $\langle \dot{\gamma}^1, \dot{\gamma}^2 \rangle = -\langle \gamma^1, \dot{\gamma}^2 \rangle$  and hence  $\langle x_\omega, x_\mu \rangle = \langle \dot{\gamma}^1, \dot{\gamma}^2 \rangle \cos^2 \omega - \langle \gamma^1, \dot{\gamma}^2 \rangle \sin^2 \omega = \langle \dot{\gamma}^1, \dot{\gamma}^2 \rangle$ .

Substitution of these results into the formula given in Corollary 1 yields

**Corollary 2.** If  $\gamma^i(\mu) \in S^{n-1}$  ( $i = 1, 2$ ) are non-selfintersecting regular  $C^3$  curves and  $\langle \gamma^1(\mu), \gamma^2(\mu) \rangle = 0$  for all  $\mu_1 \leq \mu \leq \mu_2$ , then for all  $w$  sufficiently close to 1,

$$P \left\{ \sup_{\mu_1 < \mu < \mu_2} [(\gamma^1(\mu), U)^2 + (\gamma^2(\mu), U)^2]^{1/2} > w \right\} = (1 - w^2)^{(n-2)/2} \quad (18)$$

$$+ \frac{2\Gamma(n/2)}{\pi^{3/2}\Gamma[(n-1)/2]} w(1 - w^2)^{(n-3)/2} \int_0^{\pi/2} \int_{\mu_1}^{\mu_2} [\|\dot{\gamma}^1 \cos \omega + \dot{\gamma}^2 \sin \omega\|^2 - \langle \dot{\gamma}^1, \dot{\gamma}^2 \rangle^2]^{1/2} d\mu d\omega.$$

**Remark.** Using quite different methods, Johnstone and Siegmund (1987) showed that the right hand side of (18) is an upper bound for the left hand side for all  $0 < w < 1$ . In the one dimensional case, i.e. for a tube about a curve, Johnstone and Siegmund provide two derivations of upper bounds for the tube volume which are shown to be equalities when no self overlap occurs in the tube. However, their method does not seem to yield the equality in (18), and our geometric method does not appear to give their inequality for all  $0 < w < 1$ . In fact the problem of obtaining tight upper bounds for the volume of tubes of arbitrary radii about manifolds of dimension  $\geq 2$  appears to be a difficult problem.

For a numerical example suppose that the  $t_i$  are equally spaced, so by recentering we have  $t_i = i - m$ , where  $m = (n + 1)/2$ ,  $i = 1, \dots, n$ . The model is then

$$y = \beta_1 f^1(\mu) + \beta_2 f^2(\mu) + \epsilon,$$

where  $y = (y_1, \dots, y_n)$ ,  $\epsilon = (\epsilon_1, \dots, \epsilon_n)$ ,  $f^1(\mu) = (\cos \mu(1 - m), \dots, \cos \mu(n - m))$ , and  $f^2(\mu) = (\sin \mu(1 - m), \dots, \sin \mu(n - m))$ . It is readily verified that  $\langle f^1, f^2 \rangle \equiv 0$ ,  $\|f^1\|^2 = n/2 + \sin(n\mu)/(2 \sin \mu)$ ,  $\|f^2\|^2 = n/2 - \sin(n\mu)/(2 \sin \mu)$ , and hence the  $\gamma^i$  in (17) are given by  $\gamma^i = f^i / \|f^i\|$  ( $i = 1, 2$ ). Also  $\langle \dot{\gamma}^1, \dot{\gamma}^2 \rangle \equiv 0 \equiv \langle \gamma^1, \gamma^2 \rangle$ . For  $\mu_1 = 0, \mu_2 = \pi$  the integral in (18) for our special case reduces to

$$\int_0^\pi \int_0^{2\pi} [\|\dot{\gamma}^1\|^2 \cos^2 \omega + \|\dot{\gamma}^2\|^2 \sin^2 \omega]^{1/2} d\omega d\mu. \quad (19)$$



Obtaining useful expressions for  $\|\dot{\gamma}^1\|$  and  $\|\dot{\gamma}^2\|$  requires a lengthier calculation. Some details are given by Davies (1987), who (assuming  $\sigma^2$  is known) discusses the likelihood ratio test from a different viewpoint and is led to the same integral. Davies observes that  $\|\dot{\gamma}^i(\mu)\| \sim n/(2 \cdot 3^{1/2})$  except for  $\mu$  close to 0 or  $\pi$ , which suggests use of  $\pi^2 n/3^{1/2}$  as an approximation for (19). He subsequently modifies this suggestion to be more consistent with his numerical calculations. Although the modified approximation seems excellent, in the numerical example given below we have computed (19) numerically.

For various values of  $n$  and  $w$ , Table 1 gives the right hand side of (18) and the outcome of a 10,000 repetition Monte Carlo experiment to estimate the probability on the left hand side of (18). The analytic result seems to provide a very good approximation, although it is less satisfactory for large  $n$ .

**Table 1**  
**The Probability (18)**

$n$	$w$	Right Hand Side of (18)	Monte Carlo Estimate
8	.90	.092	.091
8	.95	.018	.015
16	.75	.073	.073
16	.80	.022	.021
32	.55	.186	.181
32	.60	.058	.057
32	.65	.014	.014
64	.40	.355	.298
64	.45	.082	.069
64	.50	.014	.013

The term in Corollary 1 which involves the Euler-Poincaré characteristic of  $M$  is of smaller order of magnitude than the others as  $w \rightarrow 1$ . For manifolds of dimension  $> 2$  the analogous terms do not in general simplify as they do in the two dimensional case, and they can be quite complicated to evaluate numerically. Hence it is interesting to consider the accuracy of the approximation we obtain by simply ignoring those terms.

Our second example is concerned with essentially the same manifold  $x(\mu, \omega) = \gamma^1(\mu) \cos \omega + \gamma^2(\mu) \sin \omega$  as before, but now  $\omega$  is restricted to the range  $0 < \omega < \pi$ . The area of the new

manifold is one-half that of the old. The length of its boundary is

$$2\pi + 2 \int_0^\pi \|\dot{\gamma}^1\| d\mu,$$

and its Euler-Poincaré characteristic is one.

Table 2 gives a numerical example. The columns headed  $|M|$ ,  $|\partial M|$ , and  $\chi(M)$  give the values of the respective terms in Corollary 1. The final column gives the results of a 10,000 repetition Monte Carlo experiment.

**Table 2**  
**Effect of Neglecting the Gauss-Bonnet Term**

$n$	$w$	$ M $	$ \partial M $	$\chi(M)$	Total	Monte Carlo
8	.86	.090	.025	.001	.116	.115
8	.94	.013	.002	.000	.015	.016
16	.72	.063	.015	.001	.079	.082
16	.78	.018	.004	.000	.021	.024
32	.54	.111	.028	.001	.140	.135
32	.58	.046	.010	.000	.057	.057
64	.40	.176	.043	.000	.219	.186
64	.45	.041	.009	.000	.049	.040

The analytic result seems to be about as accurate as in the preceding example. Neglecting the term involving  $\chi(M)$  would have negligible effect, but neglecting the term involving  $|\partial M|$  would make a substantial difference. Since both  $|M|$  and  $|\partial M|$  may be shown to be proportional to  $n$ , one might have predicted these relations from analytic considerations. It is also interesting that in this case our theoretical result is not known to be an upper bound; and in three rows the Monte Carlo estimate actually exceeds slightly the theoretical value.

#### 4. Testing for a Change-point in Linear Regression.

Assume  $y_i = \beta_0 + \beta_1 t_i + \beta(t_i - \theta)^+ + \varepsilon_i$  ( $i = 1, \dots, n$ ), where the  $t_i \in [0, 1]$  are known constants  $\beta_0, \beta_1$ , and  $\beta$  are unknown parameters, and the  $\varepsilon_i$  are independent  $N(0, \sigma^2)$ . The problem of testing  $H_0 = \beta = 0$  has been discussed, for example, by Hinkley (1969, 1971), Feder (1975), and Davies (1987). Presumably one-sided alternatives, say  $H_1 : \beta > 0$ , are scientifically more relevant and we consider only this case. For our numerical examples we take the  $t_i$  to be equally spaced:  $t_i = (i - 1)/(n - 1)$ ,  $i = 1, \dots, n$ .

We begin with the special case  $\beta_0 = \beta_1 = 0$ , which fits directly into the framework of Section 1 with  $f_i(\theta) = (t_i - \theta)^+$  ( $i = 1, \dots, n$ ). Since  $\gamma(\theta) = f(\theta)/\|f(\theta)\|$  is only piecewise smooth, Hotelling's (1939) results are not directly applicable. Naiman (1986) and Johnstone and Siegmund (1987) obtain a suitable extension which gives an upper bound for the volume of the tube of geodesic radius  $\varphi$  about  $\gamma$  for all  $0 < \varphi < \pi/2$ .

We consider a slight generalization of the likelihood ratio test, where we may restrict the set over which we search for a possible change-point to a subinterval of  $[0, 1]$ , say  $[0, \theta_0]$ . (See James, James, and Siegmund, 1987, for the effect this modification has on the power of the likelihood ratio test in a related problem.) The test statistic is  $\max_{0 \leq \theta \leq \theta_0} \langle \gamma(\theta), U \rangle$  and the length of  $\gamma$  is  $|\gamma| = \int_0^{\theta_0} \|\dot{\gamma}(\theta)\| d\theta$ . According to Naiman (1986) and Johnstone and Siegmund (1987) for all  $0 < w < 1$

$$P \left\{ \max_{0 \leq \theta \leq \theta_0} \langle \gamma(\theta), U \rangle > w \right\} \leq \frac{\Gamma[n/2]}{\pi^{1/2} \Gamma[(n-1)/2]} \int_w^1 (1-x^2)^{(n-3)/2} dx + (2\pi)^{-1} |\gamma| (1-w^2)^{(n-2)/2}. \quad (20)$$

Assume now that  $t_i = (i-1)/(n-1)$  ( $i = 1, \dots, n$ ). Some calculation shows that  $\|\dot{\gamma}(\theta)\| = 0$  for  $(n-2)/(n-1) < \theta < 1$  and for  $\nu/(n-1) < \theta < (\nu+1)/(n-1)$  ( $\nu = 0, 1, \dots, n-3$ )

$$\|\dot{\gamma}(\theta)\|^2 = \left\{ \frac{(n-1-\nu)^2 - 1}{12(n-1)^2} \right\} / A_\nu^2(\theta),$$

where  $A_\nu(\theta) = \theta^2 + b_\nu \theta + c_\nu$ ,  $b_\nu = -(n+\nu)/(n-1)$ , and  $c_\nu = \{2[(n-1)^2 + 3(n-1)\nu + \nu^2] + 3(n+\nu-1) + 1\} / [6(n-1)^2]$ . It is easily checked that  $A_\nu(\theta) > 0$  for  $\nu \leq n-3$ , so

$$\int_0^{(n-1)^{-1} \lfloor (n-1)\theta_0 \rfloor} \|\dot{\gamma}(\theta)\| d\theta = \sum_{\nu=0}^m \left\{ \frac{(n-1-\nu)^2 - 1}{12(n-1)^2} \right\}^{1/2} \int_{\nu/(n-1)}^{(\nu+1)/(n-1)} d\theta / A_\nu(\theta),$$

where  $m = \min(n-3, \lfloor (n-1)\theta_0 \rfloor)$ . Integration gives

$$\begin{aligned} & \int_0^{(n-1)^{-1} \lfloor (n-1)\theta_0 \rfloor} \|\dot{\gamma}(\theta)\| d\theta \\ &= \sum_{\nu=0}^m \left\{ \tan^{-1} \left[ \frac{3^{1/2}(\nu+2-n)}{\{(n-1-\nu)^2 - 1\}^{1/2}} \right] - \tan^{-1} \left[ \frac{3^{1/2}(\nu-n)}{\{(n-1-\nu)^2 - 1\}^{1/2}} \right] \right\}. \end{aligned} \quad (21)$$

With the help of (21) one can evaluate the right hand side of (20) numerically. (Note that the first term is just  $P\{t_{n-1} \geq (n-1)^{1/2}w/(1-w^2)^{1/2}\}$ , where  $t_n$  denotes a random variable having Student's distribution with  $n$  degrees of freedom.) Some additional analysis shows that as  $n \rightarrow \infty$

$$\int_0^{\theta_0} \|\dot{\gamma}(\theta)\| d\theta \rightarrow -3^{1/2} [\log(1 - \theta_0)] / 2, \quad (22)$$

which may be used instead of (21) to evaluate approximately the right hand side of (20).

Table 3 compares the upper bound (20) with the results of a 10,000 repetition Monte Carlo experiment. Both (21) and (22) are used to evaluate the right hand side of (20), and both yield reasonably good approximations to the true probability.

**Table 3**  
**Change-point in Regression ( $\beta_0 = \beta_1 = 0$ ).**

$n$	$w$	$\theta_0$	Theory (20)		Monte Carlo
			Exact(21)	Approx. (22)	
5	.729	$(n-2)/(n-1)$	.10	.111	.095
10	.637	$(n-2)/(n-1)$	.05	.055	.049
20	.476	$(n-2)/(n-1)$	.05	.055	.047
20	.452	.80	.05	.052	.043
50	.274	$(n-2)/(n-1)$	.10	.108	.090
50	.240	.80	.10	.107	.094
50	.317	$(n-2)/(n-1)$	.05	.054	.048
50	.286	.80	.05	.054	.047

We now drop the assumption  $\beta_0 = \beta_1 = 0$ . As indicated in a slightly simpler context by Hotelling (1939)), one can reduce this case to the one considered previously as follows. Writing our model in the form  $y_i = \beta_0 + \beta_1 t_i + \beta f_i(\theta) + \varepsilon_i$  ( $i = 1, \dots, n$ ) and introducing the notation  $y = (y_1, \dots, y_n)$ ,  $t = (t_1, \dots, t_n)$ ,  $f(\theta) = (f_1(\theta), \dots, f_n(\theta))$ ,  $\varepsilon = (\varepsilon_1, \dots, \varepsilon_n)$ ,  $e = (1, \dots, 1)$ ,  $\bar{y} = n^{-1} \sum y_i$ ,  $\bar{t} = n^{-1} \sum t_i$ , and  $\bar{f}(\theta) = n^{-1} \sum f_i(\theta)$ , we let  $\tilde{y}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 t_i$ , where  $\hat{\beta}_1 = \langle t - \bar{t}e, y \rangle / \|t - \bar{t}e\|^2$  and  $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{t}$  are the maximum likelihood estimators of  $\beta_1$  and  $\beta_0$  under  $H_0 : \beta = 0$ . It is readily verified that

$$\tilde{y}_i = \beta \tilde{f}_i(\theta) + \tilde{\varepsilon}_i \quad (i = 1, \dots, n),$$

where

$$\tilde{f}_i(\theta) = f_i(\theta) - \bar{f}(\theta) - \frac{\langle t - \bar{t}e, f(\theta) \rangle}{\|t - \bar{t}e\|^2} (t_i - \bar{t})$$

and

$$\tilde{\varepsilon}_i = \varepsilon_i - \bar{\varepsilon} - \frac{\langle t - \bar{t}e, \varepsilon \rangle}{\|t - \bar{t}e\|^2} (t_i - \bar{t}).$$

Also  $\tilde{\gamma}(\theta) = \tilde{f}(\theta)/\|\tilde{f}(\theta)\|$  defines a curve on the  $n - 3$  dimensional sphere

$$\{(u_1, \dots, u_n) : \sum u_i^2 = 1, \sum u_i = 0, \sum (t_i - \bar{t})u_i = 0\},$$

and under  $H_0 : \beta = 0, \tilde{y}/\|\tilde{y}\| = \tilde{U}$  is uniformly distributed on this sphere. It follows that  $\langle \tilde{f}(\theta), y \rangle = \langle \tilde{f}(\theta), \tilde{y} \rangle$  and (20) gives an upper bound for the significance level,

$$P\left\{\max_{\theta_0 \leq \theta \leq \theta_1} \langle \tilde{\gamma}(\theta), \tilde{U} \rangle > w\right\}, \quad (23)$$

of the likelihood ratio test provided  $|\gamma|$  is replaced by  $|\tilde{\gamma}|$ , the length of the curve  $\tilde{\gamma}$ , and  $n$  is replaced by  $(n - 2)$  to account for the degrees of freedom lost in estimating  $\beta_0$  and  $\beta_1$ .

It is now in principle straightforward to evaluate the arc length of  $\tilde{\gamma}(\theta)$  and hence obtain an upper bound for (23). There does not seem to be an exact expression as simple as (21); and since (22) seemed to provide a reasonably good approximation in the previous case, we use the analogous approximation here. After substantial calculation, one finds that as  $n \rightarrow \infty$

$$\int_{\theta_0}^{\theta_1} \|\dot{\tilde{\gamma}}(\theta)\| d\theta \rightarrow (3^{1/2}/2) \log [\theta_1(1 - \theta_0)/\theta_0(1 - \theta_1)]. \quad (24)$$

Table 4 compares the analytic upper bound for (23) with the results of a 10,000 repetition Monte Carlo experiment. The analytic upper bound is given by (20) with  $n$  replaced by  $n - 2$  and  $|\gamma|$  replaced by  $|\tilde{\gamma}|$ . We have used the right hand side of (24) with  $\theta_0 = 1/(n - 1)$  and  $\theta_1 = (n - 2)/(n - 1)$  as an approximation to  $|\tilde{\gamma}|$ . For each value of  $n$  there is one Monte Carlo experiment, so the entries for fixed  $n$  and different values of  $w$  are dependent. The results indicate that except for small  $n$  the theoretical approximation is reasonable, albeit not excellent. Table 3 suggests that we could perhaps halve the error of the approximation by computing  $|\tilde{\gamma}|$  numerically.

**Table 4**  
**Change-point in Regression ( $\beta_0, \beta_1$  unknown)**

$n$	$w$	Theory	Monte Carlo
5	.963	.10	.059
5	.989	.05	.018
10	.693	.10	.080
10	.763	.05	.038
10	.867	.01	.008
20	.495	.10	.085
20	.553	.05	.043
20	.656	.01	.010
50	.321	.10	.077
50	.359	.05	.041
100	.232	.10	.079
100	.259	.05	.041

## 5. Discussion.

In this section we consider briefly some possible extensions of Theorem 2. The most obvious concerns tubes about higher dimensional manifolds (with boundary). Unfortunately there does not seem to be any way in general to avoid some nasty looking computational problems.

For example, suppose  $M$  is a three dimensional submanifold of  $S^{n-1}$  with a two dimensional boundary  $\partial M$ . It is possible for  $\partial M$  itself to have a (one-dimensional) boundary, but for simplicity we assume it does not.

The method of proof of Theorems 1 and 2 shows that the contribution to the volume of the tube of geodesic radius  $\varphi$  about  $M$  coming from points in  $S^{n-1}$  which are closest to an interior point of  $M$  is

$$V_1(\varphi) = \int_M \int_{\xi_1^2 + \dots + \xi_k^2 \leq \tan^2 \varphi} [1 + \xi_1^2(J - 3)] \frac{d\xi_1, \dots, d\xi_k}{(1 + \xi_1^2 + \dots + \xi_k^2)^{n/2}} dA.$$

Here  $k = n - 4$ ,  $dA$  is the element of surface area on  $M$ , and  $J$  is a curvature on  $M$  defined as follows. If  $(L_i^j(\nu))$  ( $\nu = 1, \dots, k+1$ ) are  $3 \times 3$  matrices defined as in (5) relative to the normals  $n(\nu)$ ,  $\nu = 1, \dots, k$ , to  $M$  in the tangent space of  $S^{n-1}$  and the normal  $n(k+1)$  to  $M$  which is

also normal to  $S^{n-1}$ , then  $J$  is the sum over  $\nu = 1, \dots, k+1$  of the sum of the three pairwise products of the eigenvalues of  $(L_i^j(\nu))$ , i.e. the second symmetric function of  $(L_i^j(\nu))$ .

The contribution to the tube volume from points closest to  $\partial M$  can be shown to equal

$$V_2(\varphi) = \int_{\partial M} \int_{\substack{\eta^2 + \xi_1^2 + \dots + \xi_k^2 \leq \tan^2 \varphi \\ \eta \leq 0}} [1 - 2\eta H_\partial(0) + \xi_1^2(K_\partial - 1)] \frac{d\eta d\xi_1^2, \dots, d\xi_k^2}{(1 + \eta^2 + \xi_1^2 + \dots + \xi_k^2)^{n/2}} dA_\partial,$$

where  $dA_\partial$  is the element of surface area on  $\partial M$ ,  $K_\partial$  is the Gaussian curvature of  $\partial M$ , and  $H_\partial(0)$  is the part of the mean curvature of  $\partial M$  associated with that normal  $n(0)$  to  $\partial M$  which lies in the tangent space of  $M$  (and points into  $M$ ).

Addition of  $V_1$  and  $V_2$  and some calculation give an expression for the volume of the tube, which involves

$$\int_M dA, \int_{\partial M} dA_\partial, \int_M J dA + 2 \int_{\partial M} H_\partial(0) dA_\partial,$$

and  $\int_{\partial M} K_\partial dA_\partial$ . The last integral can be simplified by an application of the Gauss-Bonnet Theorem. The others must be evaluated numerically in most cases. Numerical computation of the third expression appears to be rather complicated in general, although in special cases the integrands can be simplified analytically.

We are primarily interested in small probabilities, and it is easy to see that here as in Theorems 1 and 2 the terms involving curvatures of  $M$  and  $\partial M$  are of smaller order of magnitude as  $w \rightarrow 1$  than those involving the surface areas,  $|M|$  and  $|\partial M|$ . Thus we might use only these comparatively easily computed terms as an approximation. The second example in Section 3 shows that such an approximation would be quite good in that case.

We record here the first two terms of the small tube probability for an  $m$  dimensional manifold with boundary embedded in  $S^{n-1}$ . We assume  $M \subset S^{n-1}$  is defined locally by  $x = x(t)$ ,  $t \in \mathcal{T} \subset \mathbb{R}^m$ , let  $|M|$  and  $|\partial M|$  denote the surface area of  $M$  and  $\partial M$ , and let  $U$  be uniformly distributed on  $S^{n-1}$ . Then as  $w \rightarrow 1$

$$\begin{aligned} P\{\max_t \langle x(t), U \rangle > w\} &= \frac{2^{-1} \Gamma(n/2) |M|}{\pi^{(m+1)/2} \Gamma[(n-m+1)/2]} w^{m-1} (1-w^2)^{(n-m-1)/2} \\ &+ \frac{4^{-1} \Gamma(n/2) |\partial M|}{\pi^{m/2} \Gamma[(n-m+1)/2]} w^{m-2} (1-w^2)^{(n-m)/2} + O((1-w^2)^{(n-M+1)/2}). \end{aligned} \quad (25)$$

Complete development of these ideas is a project for future research. See Naiman (1987) for a theoretical beginning in this direction and Johansen and Johnstone (1988) for a thought provoking application.

Naiman (1986) and Johnstone and Siegmund (1987) show that Hotelling's formula giving the exact volume of a tube of small radius about a non-closed curve actually provides an

upper bound for the volume of a tube of arbitrary radius. (The result also applies to closed curves provided they are given fictitious end points and regarded as not closed.) It would be interesting to obtain good upper bounds for the volume of tubes of arbitrary radii about higher dimensional manifolds. However, simple examples of surfaces in  $\mathbb{R}^3$  show that the situation is much more complicated than for curves. In particular, for a cylinder of unit radius and height  $h$  the formula for the volume of tube of radius  $a < 1$ , to wit  $4\pi ah + 2\pi^2 a^2$ , does not give an upper bound for the volume of a tube of radius  $a > 1$  when  $h$  is large. On the other hand the formula for the volume of a tube of radius  $a < 1$  about  $S^2 \subset \mathbb{R}^3$ ,  $8\pi a(1 + a^2/3)$ , provides an upper bound for the volume for all  $a$  although for  $S^1 \subset \mathbb{R}^2$  the closed curve must be given fictitious endpoints in order to obtain an upper bound valid for tubes of large radii.

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## References

- Davies, Robert B. (1987). Hypothesis testing when a nuisance parameter is present only under the alternative, *Biometrika* **74**, 33-43.
- Do Carmo, M. (1976). *Differential Geometry of Curves and Surfaces*, Prentice Hall, Englewood Cliffs.
- Fedler, P. (1975). The log likelihood ratio in segmented regression, *Ann. Statist.* **3**, 84-97.
- Gray, A. (1982). Comparison theorems for the volumes of tubes as generalizations of the Weyl tube formula, *Topology* **21**, 201-228.
- Griffiths, P. A. (1978). Complex differential and integral geometry and curvature integrals associated to singularities of complex analytic varieties, *Duke Math. J.* **45**, 427-512.
- Hinkley, D. V. (1969). Inference about the intersection in two-phase regression, *Biometrika* **56**, 495-504.
- Hinkley, D. V. (1971). Inference in two-phase regression, *Jour. Amer. Statist. Assoc.* **66**, 736-743.
- Hotelling, H. (1939). Tubes and spheres in  $n$ -space a class of statistical problems, *Amer. J. Math.* **61**, 440-460.
- James, B., James, K. L., and Siegmund, D. (1987). Tests for a change-point, *Biometrika* **74**, 71-84.
- Johansen, Søren and Johnstone, Iain (1988). Hotelling's theorem on the volume of tubes: some illustrations in simultaneous inference and data analysis, unpublished manuscript.
- Johnstone, Iain and Siegmund, David (1987). On Hotelling's formula for the volume of tubes and Naiman's inequality, unpublished manuscript.
- Knowles, M. (1987). Simultaneous confidence bands for random functions. Stanford University Ph.D. Thesis.
- Langevin, R. and Shifrin, T. (1982). Polar varieties and integral geometry, *Amer. J. Math.* **104**, 553-605.
- Milman, R. S. and Parker, G. D. (1977). *Elements of Differential Geometry*, Prentice Hall, Englewood Cliffs.

Naiman, D. Q. (1986a). Conservative confidence bands in curvilinear regression, *Ann. Statist.* **14**, 896-906.

Naiman, D. Q. (1986b). Simultaneous confidence bands in multiple regression using predictor variables constraints, *Jour. Amer. Statist. Assoc.* **82**, 214-219.

Naiman, D. Q. (1987). Simultaneous confidence bands for response surfaces and volumes for tubular neighborhoods of spherical polyhedra, unpublished manuscript.

Weyl, H. (1939). On the volume of tubes, *Amer. J. Math.* **61**, 461-472.

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